

# 3-Methylbut-2-enoic acid, 2-methylpentyl ester

<b>Inchi:</b>	InChI=1S/C11H20O2/c1-5-6-10(4)8-13-11(12)7-9(2)3/h7,10H,5-6,8H2,1-4H3
<b>InchiKey:</b>	GWLJUFYIQMBWFI-UHFFFAOYSA-N
<b>Formula:</b>	C11H20O2
<b>SMILES:</b>	CCCC(C)COC(=O)C=C(C)C
<b>Mol. weight [g/mol]:</b>	184.28

## Physical Properties

Property code	Value	Unit	Source
gf	-122.95	kJ/mol	Joback Method
hf	-413.02	kJ/mol	Joback Method
hfus	22.40	kJ/mol	Joback Method
hvap	48.89	kJ/mol	Joback Method
log10ws	-2.90		Crippen Method
logp	2.932		Crippen Method
mcvol	168.990	ml/mol	McGowan Method
pc	2137.41	kPa	Joback Method
rinpol	1270.00		NIST Webbook
tb	530.97	K	Joback Method
tc	715.64	K	Joback Method
tf	251.85	K	Joback Method
vc	0.650	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	397.44	J/molxK	530.97	Joback Method
cpg	412.62	J/molxK	561.75	Joback Method
cpg	427.13	J/molxK	592.53	Joback Method
cpg	440.98	J/molxK	623.31	Joback Method
cpg	454.19	J/molxK	654.08	Joback Method
cpg	466.77	J/molxK	684.86	Joback Method
cpg	478.75	J/molxK	715.64	Joback Method

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U355128&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U355128&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>

# Legend

<b>cpg:</b>	Ideal gas heat capacity
<b>gf:</b>	Standard Gibbs free energy of formation
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfus:</b>	Enthalpy of fusion at standard conditions
<b>hvap:</b>	Enthalpy of vaporization at standard conditions
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>rinpola:</b>	Non-polar retention indices
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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